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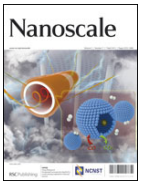

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Confinement effects and why carbon nanotube bundles can work as gas sensors †

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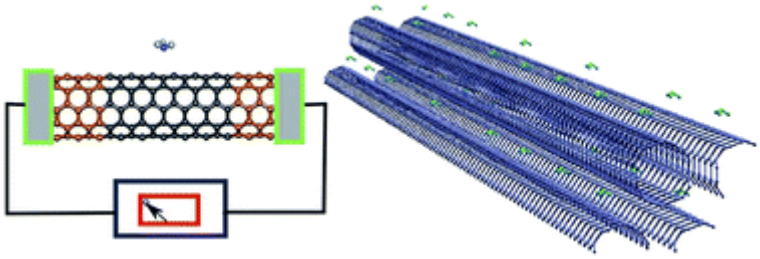
Abstract

Carbon nanotubes have been at the forefront of nanotechnology, leading not only to a better understanding of the basic properties of charge transport in one dimensional materials, but also to the perspective of a variety of possible applications, including highly sensitive sensors. Practical issues, however, have led to the use of bundles of nanotubes in devices, instead of isolated single nanotubes. From a theoretical perspective, the understanding of charge transport in such bundles, and how it is affected by the adsorption of molecules, has been very limited, one of the reasons being the sheer size of the calculations. A frequent option has been the extrapolation of knowledge gained from single tubes to the properties of bundles. In the present work we show that such procedure is not correct, and that there are qualitative differences in the effects caused by molecules on the charge transport in bundles *versus* isolated nanotubes. Using a combination of density functional theory and recursive Green's function techniques we show that the adsorption of molecules randomly distributed onto the walls of carbon nanotube bundles leads to changes in the charge density and consequently to significant alterations in the conductance even in pristine tubes. We show that this effect is driven by confinement which is not present in isolated nanotubes. Furthermore, a low concentration of dopants randomly adsorbed along a two-hundred nm long bundle drives a change in the transport regime; from ballistic to diffusive, which can account for the high sensitivity to different molecules.



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